What is Claimed is:

1. A computer-based method for facilitating the selection of chemical compounds, comprising:

receiving an identification of a target compound and a neighborhood range from a user;

performing a chemical similarity join to identify compounds of interest within said neighborhood range of said target compound; and

providing results of said chemical similarity join to the user.

2. The method of claim 2, further comprising the step of estimating properties of said target compound from properties of said compounds identified by said chemical similarity join.

3. The method of claim 1, wherein said identification of said target compound comprises an identification of a chemical structure of said target compound.

4. The method of claim 1, wherein said neighborhood range comprises a range of values of property metrics for said target compound.

5. The method of claim 1, wherein said neighborhood range comprises at least one of the group of a range of chemistry space surrounding said target compound and a cell-based neighborhood in which said target compound resides.

6. The method of claim 1, wherein said step of performing a chemical similarity join comprises the step of determining similarities between

compounds to determine whether a compound is within said neighborhood range.

7. The method of claim 6, wherein said similarities are determined using at least one of the group of Tanimoto coefficients and Molecular holograms.

8. The method of claim 1, wherein communication with said user is performed via the Internet.

9. The method of claim 1, further comprising the step of eliminating one or more compounds from consideration based on user-defined criteria for a non-desirable compound.